02-03-03

GP 2863

**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

IN RE:

| | | |
|---|---|---|
| APPLICATION OF | : | Richard Cramer, Robert Jilek, Qian Liu, Stefan Güessregen, Bernd Wendt, and Katherine Andrews |
| TITLE | : | A Method For Searching Heterogenous Compound Databases Using Topomeric Shape Descriptors and Pharmacophoric Features |
| SERIAL NO. | : | 09/825,448 |
| FILING DATE | : | April 2, 2001 |
| ART UNIT | : | 2863 |
| EXAMINER | ; | Anthony T. Dougherty |
| ATTORNEY DOCKET NO. | : | 3017-40 |



TO: Assistant Commissioner for Patents
Washington, DC 20231

Dear Sir:

Transmitted for filing in the above identified application are the following documents:

1. Response to Office Action dated July 31, 2003
2. *Petition for Extension of Time* with attached check in the amount of $465;
3. a substitute page 2 of the specification with required correction and a marked up page showing the correction made;
4. a return postcard; and
5. an Express Mail certification.

Please address all correspondence regarding this patent application to me at the address set out below.

January 31, 2003

Respectfully submitted,

Laurence Weinberger

Enclosures

Laurence A. Weinberger
Attorney for Applicants
USPTO Reg. No. 27,965

Express Mail No. ET801455699US

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**EXPRESS MAIL FILING**

Express Mail Mailing Label No.: **ET801455699US**

Date Of Deposit: January 31, 2003

I hereby certify that this paper or fee is being deposited with the United States Postal Service "EXPRESS MAIL POST OFFICE TO ADDRESSEE" service under 37 CFR 1.10 on the date indicated above and is addressed to Assistant Commissioner for Patents, Washington, D.C. 20231.

Laurence Weinberger

Laurence A. Weinberger

#7/Response
2/11/03

Express Mail No. ET801455699US

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TO: Assistant Commissioner for Patents
Washington, DC 20231

Response To Office Action Dated July 31, 2002

Dear Sir:

Applicants hereby respond to the Office Action dated July 31, 2002 in which the Examiner raised an objection to the application and rejected the claims.

Objection Response:

The Examiner has objected to an informality on page 2, line 12 with respect to an open parenthesis. Attached to this response is a substitute page 2 with a corrected parenthetical expression set out on line 12.

Rejection Response:

The Examiner has rejected claims 1 and 2 under 35 U.S.C. §102(e) as being anticipated by U.S. Patent No. 6,240,374 to Cramer et al. The Examiner states that:

> "With regard to independent method claim 1, Cramer et al. clearly shows defining fragments of a query molecule and database molecules according to a defined set of rules, generating shape descriptors, and using the shape descriptors to identify a database molecule with a shape similar to the query molecule (see column 74 line 42 through column 75 line 10)."

Applicants respectfully disagree with the Examiner's characterization of the Cramer et al. disclosure. Applicants respectfully submit that the Examiner has misinterpreted the Cramer disclosure. First it should be noted that in the present application, a database molecule is one found in a heterogenous database of actually existing molecules such as those available commercially. (See first full paragraph on page 6). The database contains the description of each molecule, not its constituent parts. There is simply no equivalent database of existing molecules taught in Cramer.

The Examiner is correct that Cramer does teach the fragmentation of a query molecule and characterization of the fragments by shape descriptors. However, since there is no database of heterogenous molecules in Cramer, Cramer can not and does not teach the fragmentation of a database molecule or molecules from a heterogenous database. Rather, in Cramer, a Virtual Library was constructed consisting of structural variations (component parts) which might be combinatorially assembled into a molecule by known synthetic routes. Associated with the structural variations in the Virtual Library were their descriptions in terms of molecular

structural metrics. The Virtual Library could be searched for product molecules possessing desired shape characteristics without the actual generation of the molecular structure of the products by the computer in order to accomplish the search. This is what is described in the Examiner's citation to column 74, lines 42-48:

> As described earlier, the topomeric 3D shape data within the Virtual Library actually describe fragments (structural variations) of molecules. To find similarly shaped molecules within the virtual library, the query molecule must be fragmented and the shapes of its fragments compared with the shapes of corresponding fragments (structural variations) in the virtual library. Column 74, lines 42 - 48.

Clearly the method of the present application is not disclosed or taught by the Cramer et al. patent.

The Examiner further states that:

> "With regard to independent method claim 2, Cramer et al. clearly shows fragmenting query and database molecules, generating topomeric conformations and interaction energies of query and database molecules and determining similarity by root sum square to identify a molecule in the database most similar to the query molecule (see column 73 line 50 through column 75 line 10).

As noted above, since there is no database of heterogenous molecules in Cramer, Cramer can not and does not teach the fragmentation of a heterogenous database molecule or molecules. The Examiner's statement is in error. It should also be noted that neither Cramer nor the present application teach "..generating topomeric conformations and interaction energies of query and database molecules..." as noted by the Examiner. The present application does teach generating

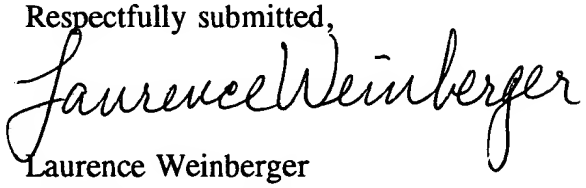
topomeric conformations and interaction energies of fragments derived from query and database molecules.

For the above reasons, Applicants submit that the Cramer et al. patent does not anticipate the invention of the present application. Applicants respectfully request that the Examiner withdraw the rejections under 35 U.S.C. §102(e) and permit the patent to issue.

Double Patenting Response:

The Examiner has rejected claims 1 and 2 under the judicially created doctrine of obviousness-type double patenting "...as being unpatentable over claim 3 of U.S. Patent 6,240,374." While the Examiner notes that the claims are not identical, he suggests that they are not patentably distinct from each other. Applicants believe the Examiner has come to this conclusion due to the same misreading of the Cramer patent as discussed above. Claim 3 of the Cramer patent does not teach the search of molecules in a heterogeneous database for molecules similar to a query molecule. Claim 3 of Cramer is directed to identifying in a Virtual Library of structural variations, product molecules which might be assembled from the structural variations which would have a shape similarity to the query molecule. No fragmenting of molecules in a heterogenous database of actual molecules is taught by Cramer. Accordingly, Applicants respectfully request that the Examiner withdraw the double patenting rejection and permit the patent to issue.

Respectfully submitted,



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